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A study of electron production in proton-biomolecule collisions using additivity rules

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Synopsis Additivity rules are employed to estimate electron production cross sections for proton collisions with nucleobases and amino acids at collision energies 10 keV$\leq E \leq$2 MeV. Total and differential cross sections agree with the available theoretical and experimental cross sections, and the method can be easily applied to estimate electron production cross sections for collisions with other biomolecules.

Electron production (EP) in proton-molecule collisions takes place through the reactions:

$$H^+ + M \rightarrow ne^- + H^{(1-m)+} + M^{(n+m)+}, \quad (1)$$

where M is the target molecule, $m = 0, 1$ and $n \geq 1$. These processes are relevant in cancer proton therapy (see e.g., [1]), where high energy protons give rise to the ionization and ensuing fragmentation of the biomolecules.

In this work we present a semiempirical treatment to estimate the EP total and differential cross sections by employing additivity rules that combine the cross section for atoms and small molecules. This simple approach yields results in good agreement with existing experimental and theoretical values in a wide collision energy range that includes low collision energies, where perturbative calculations are not appropriate. The method can be easily applied to many collisions, provided that the cross sections for the small molecules involved in the additivity rules are available. As an illustration, we show in Fig. 1 our estimates of the single differential, in electron energy, cross sections (SDCS), σ^ϵ, for proton collisions with uracil and adenine. We have used the additivity rules:

$$\sigma^\epsilon(\text{Base}) = a_1\sigma^\epsilon(CO_2) + a_2\sigma^\epsilon(O_2) + a_3\sigma^\epsilon(N_2) + a_4\sigma^\epsilon(H_2) \quad (2)$$

where the SDCS for collisions with CO_2, O_2, N_2 and H_2 are the experimental values [2], and the coefficients a_i are determined by the molecular formulae of the nucleobases. One can note the excellent agreement between our values and those from the CB1 calculations. The disagreement between theoretical and experimental results at $\epsilon < 7$ eV remains unexplained. The "humps" in the experimental curves might arise from interference effects between collisions with different atoms, although a similar decrease of the experimental SDCS has not been observed in proton collisions with small molecules.

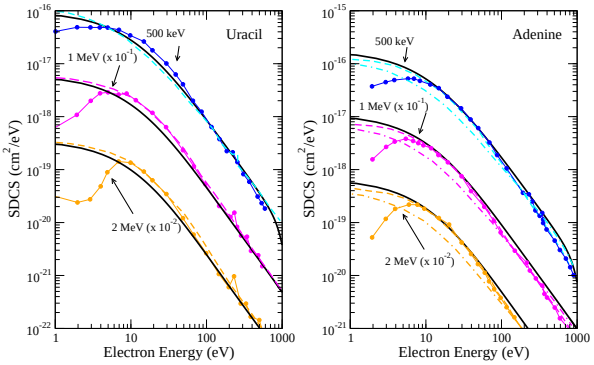

Figure 1. SDCS for EP in proton collisions with uracil and adenine, as functions of the energy of the emitted electron. The full lines are the present results from eq. (2). Dashed lines, first Born approximation with corrected boundary conditions (CB1) calculations [3, 4]; dashed-dotted lines in the right panel, continuum distorted wave-eikonal initial state (CDW-EIS) approximations [4]. Lines with circles, experimental results of references [3] (H^+ + uracil) and [5] (H^+ + adenine).

References

[1] D. Schardt *et al* 2010 *Rev. Mod. Phys.* **82** 383

[2] M. E. Rudd *et al* 1992 *Rev. Mod. Phys.* **64** 441

[3] A. Itoh *et al* 2013 *Phys. Rev. A* **88** 052711

[4] M. E. Galassi *et al* 2012 *Phys. Med. Biol* **57** 2081

[5] Y. Iriki *et al* 2011 *Phys. Rev. A* **84** 052719

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